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-Technical Report-

Near Infrared Fuel Analyzer Temperature Evaluation

Joel Schmitigal

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Near Infrared Fuel Analyzer Temperature Evaluation

Joel Schmitigal
Force Projection Technology

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1. **Introduction**

The objective of this effort was to evaluate the portable Near Infrared (NIR) Spectrometer fuel analyzer, FuelEX by Bruker Optics Inc., developed under guidance from TARDEC under Small Business Innovative Research contract DAAE07-01-C-L008, to the temperature testing requirements set forth in the draft performance specification for the instrument. The Spectrometer evaluated under this effort were received by TARDEC under contract W56HZV-08-C-L534, an effort that ruggedized the instrument to meet the Army's environmental requirements. The NIR spectrometer is being developed for utilization in the Army's Petroleum Test Kit, which will provide fuel handlers with a last quality check of the fuels usability, including fuel type, before vehicle or aircraft fueling.

The FuelEX NIR spectrometer utilizes Partial Least Squares (PLS) chemometrics to predict the properties of the fuel and determines the usability of the fuel based on these values as has been detailed in previous reports (1) (2) (3) (4) (5).

2. **Approach**

The NIR fuel analyzer temperature tests were performed to evaluate the repeatability of a single instrument across a temperature range of -35°C to 58°C as specified in the Petroluem Test Kit's (PTK) draft Capabilities Production Document (CPD) (6). The PTK Operational Requirements Document (ORD) (7) had previously stated temperature requirements to be -35°C to 58°C.

The test procedure subjected the analyzer and a series of nine jet fuels (Table 1) to a temperature of -35 ± 2 °C for a period of 4 hours. The nine fuels were then tested by the spectrometer. Kerosene based aviation fuels were utilized due to Diesel No. 2 fuels having a cloud point higher than -18°C. For consistency in reporting the fuels used in this evaluation were previously evaluated to determine the instrument's repeatability and reproducibility and compared to ASTM test values (1). This procedure was then repeated at temperatures of -18 ± 2 °C, 0 ± 2 °C, 21 ± 2 °C, 27 ± 2 °C, 39 ± 2 °C, 49 ± 2 °C, 58 ± 2 °C.

Prior to sampling being performed at each temperature set point, the instrument was powered up and a quick calibration was performed which utilizes reagent grade heptane to calibrate the x-axis. Baseline effects were removed from all spectra using a 7pt Savitsky-Golay 1st derivative followed by a standard normal variate (SNV) transform. The SNV transform is applied to the spectra by subtracting the spectral mean from the spectrum then dividing by the spectral standard deviation of the spectrum.

Sample ID	Fuel Type
740	JP-8
890	JP-8
1041	JP-8
1238	JP-5
12988	JP-8
12996	JP-8
13141	JP-8
13301	JP-8
13344	JP-8

Table 1. Test Fuels

3. **Analysis**

3.1. Spectra comparison

The raw fuel spectra were analyzed to determine if the fuel and instrument temperature variations had an effect on the fuel spectra. The raw spectral data (Figure 1) exhibited significant baseline variations as is commonly seen when collecting NIR data. Spectral shifts can be easily observed when the baseline variations were removed from the spectra using the 7pt Savitsky-Golay 1st derivative and SNV transform (Figure 2). Close analysis of these shifts (in this instance of wavelengths between 1394-1401 nm) is shown in Figure 3. Spectral shifts are shown to be a direct result of temperature variation.

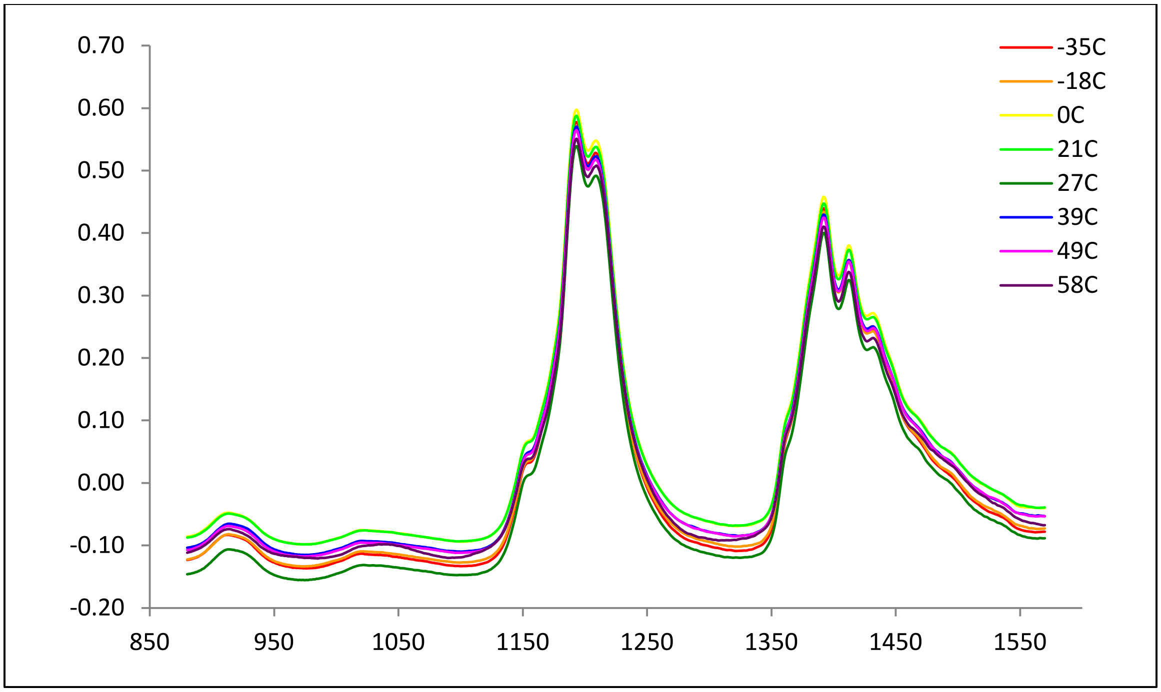

Figure 1. The raw spectral data shows significant baseline variations as is commonly with NIR data.

Figure 2. Fuel spectra normalized utilizing a 7pt Savitsky-Golay 1st derivative followed by a standard normal variate (SNV) transform display spectral shifts caused by temperature.

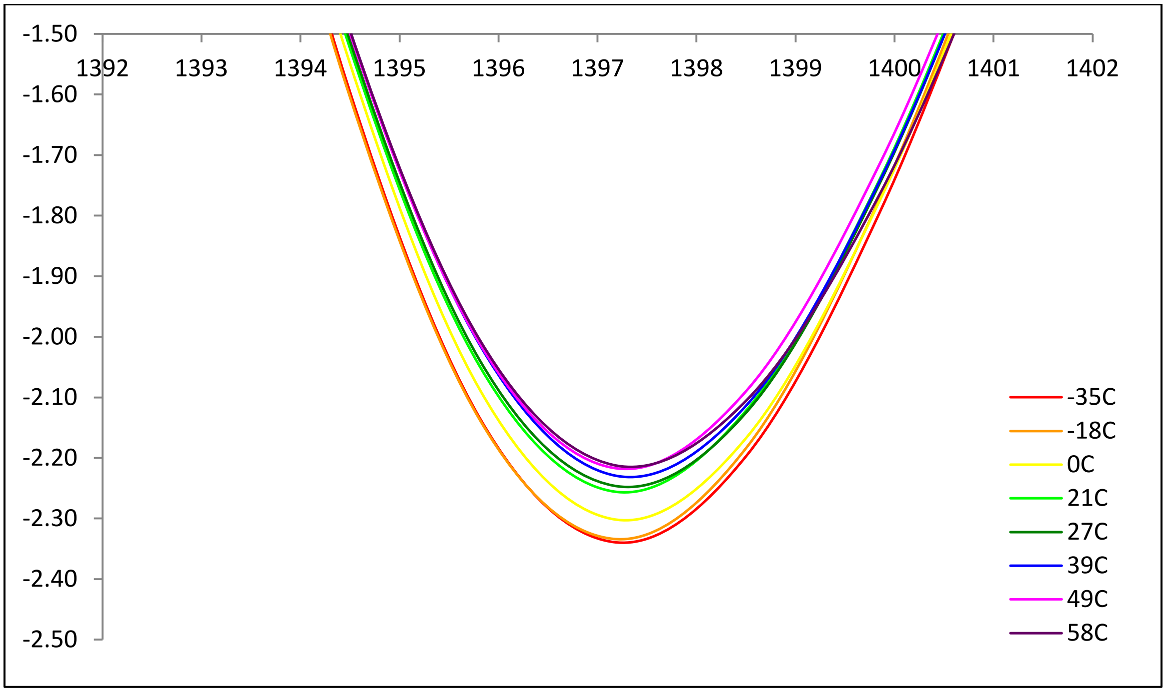

Figure 3. Spectral shifts direct resulting from temperature variation shown in spectra in the 1394-1401 nm wavelength region.

3.2. Fuel Property Prediction

The nine fuel samples tested where found to be on specification for all properties at all test points though out the temperature range. A drift in predicted properties was identified in all 11 properties that were predicted utilizing chemometic models (Appendix A). In all instances the spectral drift caused a linear, or near linear, (Appendix B) drift in the predicted property result which corresponds to the spectrial shifts shown in Figures 2 and 3.

As all fuel models were built off of spectra taken at 21°C the drift in the predicted property result minimizes the error attributable to the spectral drift across the required temperature requirement of the instrument. In no instance did the drift in property prediction of the 9 fuels analyzed cause them to fall out of specification. As evidenced by displayed drift, it is possible that a fuel that would be predicted as on specification at temperature X may be predicted as off specification at temperature Y. This effect would need to be taken into account when setting acceptable limits beyond strict limits at traditionally established manufacture or military specification limits for fuels.

The repeatability of the instrument through the temperature range of test showed that the fuel analyzer and chemometic models had a slightly higher repeatability, but still compared well to that of the published values of the standard ASTM measurement practices (8) (9) (10) (11) (12) (13) (14), as shown in Table 2. NIR repeatability was calculated using 95% probability and average standard deviation of the 8 measurements taken of each of the 9 jet fuel samples measured with the same instrument over the test temperature range.

Property		Average NIR Standard Deviation	NIR Repeatability	ASTM Repeatability
Density	(g/mL)	0.00096	0.0025	0.0005
Cetane Index		0.6	1.6	N/A
Aromatics	(%)	0.5	1.2	1.4
Distil. 10%	(°C)	2.5	6.5	1.9-3.7
Distil. 90%	(°C)	2.1	5.5	2.1-2.9
Flash Point	(°C)	1.7	4.5	1.2-2.3
Freeze Point	(°C)	0.94	2.44	0.54
Viscosity -20°C	(cSt)	0.11	0.30	0.03

Table 2.NIR Repeatability of Jet fuel models.
Calculated using 95% probability and average standard deviation of the 8 measurements taken of each of the 9 jet fuel samples measured with the same instrument over the test temperature range. ASTM values taken, or derived, from ASTM method documents (www.astm.org).

4. **Conclusion**

The analysis of the NIR fuel analyzer against the required environmental temperature range required by a field portable instrument by the U.S. Army showed that the instrument and technology is capable of performing its function from a temperature of -35°C to 58°C. The shifts observed in the fuel spectra show a direct correlation to temperature variation, but the resulting drift in the predicted fuel properties are not larger than the error associated with the instrumentation and ASTM methods that it correlates to. This should be recognized when establishing fuel use restrictions for the fielded instrument in that it would be prudent to set acceptable limits beyond the strict manufacture and use thresholds established for fuels.

References

1. **Schmitigal, Joel.** *Near-Infrared Spectroscopy and Chemometrics Instrumention and Methodology for Field Evaluation of Diesel and Aviation Fuels by the U.S. Army.* Warren : TARDEC, 2010.
2. *Design Improvements for the Army Portable NIR Fuel Analyzer.* **Cooper, John and Schmitigal, Joel.** New Orleans : Coordinating Research Council Inc., 2009.
3. *New Capabilities and Future Directions for the FUELex Portable Fuel Analyzer.* **Cooper, John and Schmitigal, Joel.** Alexandria : Coordinating Research Council Inc, 2010.
4. *Portable Fuel Analyzer for the Army Petroleum Test Kit: Current Design and Future Goals.* **Cooper, John and Schmitigal, Joel.** Alexandria : Coordinating Research Council, 2008.
5. *Near-Infrared Fuel Analysis.* **Schmitigal, Joel.** Alexandria : Coordinating Research Council, 2006.
6. Capability Production Document For The Petroleum Test Kit (PTK) (DRAFT V. 1.0). 2008.
7. Operational Requirements Document for Petroleum Test Kit (PTK) ACAT III. December 11, 2002.
8. *Standard Test Method for Density, Relative Density (Specific.* West Conshohocken : American Society of Testing and Materials, 1999. ASTM D 1298-99.
9. *Standard Test Method for Calculated Cetane Index by Four Variable Equation.* West Conshohocken : American Society of Testing and Materials, 2009. ASTM D 4737-09.
10. *Standard Test Method for Hydrocarbon Types in Liquid Petroleum Products by Fluorescent Indicator Adsorption.* West Conshohocken : American Society of Testing and Materials, 2010. ASTM D1319-10.
11. *Standard Test Method for Distillation of Petroleum Products at Atmospheric Pressure.* West Conshohocken : American Society of Testing and Materials, 2009. ASTM D 86-09.
12. *Standard Test Methods for Flash Point by Pensky-Martens Closed Cup Tester.* West Conshohocken : American Society of Testing and Materials, 2010. ASTM D 93-10.
13. *Standard Test Method for Freezing Point of Aviation Fuels (Automatic Phase Transition Method).* West Conshohocken : American Society of Testing and Materials, 2010. ASTM D 5972-05.
14. *Standard Test Method for Kinematic Viscosity of Transparent and Opaque Liquids (and Calculation of Dynamic Viscosity).* West Conshohocken : American Society of Testing and Materials, 2009. ASTM D 445-09.
15. *Standard Test Method for Cloud Point of Petroleum Products.* West Conshohocken : American Society of Testing and Materials, 2009. ASTM D 2005-09.

Appendix A

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	14.9	14.2	13.5	13.7	13.6	13.5	13.6	13.4
Cetane Index	48.5	48.2	48.3	47.9	48.1	47.8	47.3	46.7
Density (g/mL)	0.8006	0.7992	0.7993	0.7993	0.7992	0.7997	0.7995	0.8021
Distil. 10% (°C)	176.8	175.9	175.5	176.4	176.2	179.9	179.2	181
Distil. 20% (°C)	184.6	183	183.1	183.8	183.7	187.1	185.8	188.2
Distil. 50% (°C)	207	205.2	205	205.1	204.9	207.4	206.2	207.9
Distil. 90% (°C)	243.9	242	240.6	238.9	239.1	238.2	238.1	237.6
Flash Point (°C)	46.7	46.7	45.7	46.6	46.7	49	48.7	50
Freeze Point (°C)	-51.5	-52.6	-53	-52.8	-52.9	-52.5	-52.4	-50
H-Content (%)	13.9	14	14	14	14	14	14	13.9
Viscosity -20°C (cSt)	4.7	4.6	4.5	4.4	4.4	4.4	4.3	4.5

Table A1. Chemometic model data output for Jet fuel 13344 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	14.8	14	13.7	13.7	13.6	13.4	13.5	13.1
Cetane Index	47.9	47.4	47.8	47.2	47.3	47.2	46.3	46.2
Density (g/mL)	0.8007	0.7988	0.7997	0.7996	0.7994	0.8001	0.7997	0.8016
Distil. 10% (°C)	174.3	173	174.6	175.2	174.2	177.3	176.8	179.8
Distil. 20% (°C)	181.8	179.8	182	182.2	181.4	184.3	182.9	186.4
Distil. 50% (°C)	204.9	202.6	204.3	204.1	203.3	205.3	204	206.9
Distil. 90% (°C)	243.5	241.2	240.5	239.1	238.7	238.1	237.5	237.2
Flash Point (°C)	45.3	45.4	45.6	46.3	45.7	47.8	47.7	49.5
Freeze Point (°C)	-52.7	-54.2	-53.8	-53.7	-54	-53.6	-53.7	-51.8
H-Content (%)	13.9	14	14	14	14	14	14	13.9
Viscosity -20°C (cSt)	4.6	4.4	4.4	4.3	4.3	4.3	4.2	4.3

Table A2. Chemometic model data output for Jet fuel 13301 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	19.1	18.3	18	17.9	17.9	17.5	17.5	17.5
Cetane Index	45.6	45.2	45.6	44.8	45	44.8	44.1	43.9
Density (g/mL)	0.8013	0.7992	0.7998	0.8002	0.8002	0.8004	0.8004	0.8026
Distil. 10% (°C)	179	177.1	177	180.4	178.4	182.3	182.3	184.9
Distil. 20% (°C)	186.4	183.7	184.3	187.1	185.4	188.9	188.1	191.3
Distil. 50% (°C)	206.5	203.6	204.1	205.7	204.3	206.7	206	208.6
Distil. 90% (°C)	243.9	241.3	240.4	238.6	238.6	238	237.4	237.3
Flash Point (°C)	49.9	49.5	48.6	51.1	50.1	52.4	52.4	54.4
Freeze Point (°C)	-48.5	-50.2	-50.2	-49.7	-50.1	-49.4	-49.5	-47.4
H-Content (%)	13.8	13.8	13.8	13.8	13.8	13.8	13.8	13.8
Viscosity -20°C (cSt)	4.4	4.3	4.2	4.1	4.2	4.2	4.1	4.2

Table A3. Chemometic model data output for Jet fuel 13141 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	16.7	16.8	16.5	16.6	16.3	16.1	16.1	16.2
Cetane Index	43.7	43.2	43.6	43.2	43.3	43	42.2	42
Density (g/mL)	0.8057	0.8043	0.8053	0.8052	0.8048	0.8053	0.805	0.8081
Distil. 10% (°C)	179.7	176.7	179.4	179.8	179	182.4	181.8	184.4
Distil. 20% (°C)	186.7	183.1	186.2	186.3	185.6	188.8	187.4	190.8
Distil. 50% (°C)	207	204	206.4	206.1	205.3	207.6	206.4	209.1
Distil. 90% (°C)	241.6	241.9	241	239.4	239	238.2	237.7	237.9
Flash Point (°C)	50.8	49.8	50.6	51.2	50.9	53.1	52.7	54.7
Freeze Point (°C)	-50.7	-51.4	-50.8	-50.9	-51.2	-50.7	-50.8	-48.1
H-Content (%)	13.8	13.8	13.8	13.8	13.8	13.8	13.8	13.8
Viscosity -20°C (cSt)	4.5	4.5	4.4	4.3	4.3	4.3	4.3	4.5

Table A4. Chemometic model data output for Jet fuel 12996 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	17.5	16.7	16.5	16.6	16.3	16.3	16.1	16.2
Cetane Index	44.5	43.7	44.2	43.7	43.8	43.8	42.9	42.7
Density (g/mL)	0.8061	0.8043	0.8054	0.8055	0.8048	0.8054	0.8051	0.8077
Distil. 10% (°C)	179.3	178.7	181.5	182.6	181.3	184.1	184	185.7
Distil. 20% (°C)	186.8	185.1	188.6	189.4	188.1	190.7	189.8	192.4
Distil. 50% (°C)	207.8	205.7	208.3	208.6	207.3	209.1	208.3	210.2
Distil. 90% (°C)	244.2	242	241.5	239.8	239.4	238.8	238.3	238
Flash Point (°C)	50.1	50.7	51.5	52.8	52.1	53.9	53.9	55.3
Freeze Point (°C)	-49.1	-50.6	-50.1	-50	-50.3	-49.7	-49.7	-47.3
H-Content (%)	13.8	13.8	13.8	13.8	13.8	13.8	13.8	13.8
Viscosity -20°C (cSt)	4.7	4.5	4.5	4.4	4.4	4.4	4.3	4.6

Table A5. Chemometic model data output for Jet fuel 12988 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	18.6	17.8	17.5	17.6	17.3	17.3	17.4	17.1
Cetane Index	48	47.6	47.8	47.3	47.3	47.4	46.3	46.2
Density (g/mL)	0.7981	0.7966	0.7974	0.7975	0.7972	0.7978	0.7976	0.7992
Distil. 10% (°C)	184.3	182.3	184.8	186.2	184.2	188.1	187.9	190.5
Distil. 20% (°C)	192	189.4	192.1	193.1	191.3	195	193.8	196.9
Distil. 50% (°C)	210.2	207.5	209.3	209.8	208.3	211	209.6	212.3
Distil. 90% (°C)	243.3	241	239.8	238.8	238.2	238	236.7	236.9
Flash Point (°C)	52.6	51.9	52.9	54.4	53.3	55.6	55.9	57.4
Freeze Point (°C)	-46.2	-47.5	-47.5	-47.3	-47.8	-47.1	-47.5	-45.7
H-Content (%)	13.9	13.9	13.9	13.9	13.9	13.9	13.9	13.9
Viscosity -20°C (cSt)	4.6	4.5	4.4	4.3	4.3	4.3	4.2	4.3

Table A6. Chemometic model data output for Jet fuel 1238 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	21.4	20.9	20.6	20.4	20.2	20	20.5	19.9
Cetane Index	41.6	41.4	41.5	41	41.2	40.9	40.3	39.7
Density (g/mL)	0.8064	0.805	0.806	0.8058	0.8055	0.8061	0.806	0.8082
Distil. 10% (°C)	166.7	165.4	167.7	168.1	166.8	170.8	170.6	173
Distil. 20% (°C)	174.5	172.7	175.3	175.5	174.3	177.9	177	179.9
Distil. 50% (°C)	198.3	196.2	198.1	197.8	196.8	199.4	198.7	200.8
Distil. 90% (°C)	245.6	243.6	242.5	240.8	240.5	239.9	239.9	239.1
Flash Point (°C)	44.3	44.2	45	45.5	44.9	47.3	47.5	49.1
Freeze Point (°C)	-52.7	-54.1	-53.9	-53.9	-54.2	-53.6	-53.4	-51.1
H-Content (%)	13.6	13.6	13.6	13.6	13.6	13.6	13.6	13.6
Viscosity -20°C (cSt)	4.1	4	4	3.9	3.9	3.9	3.8	4

Table A7. Chemometic model data output for Jet fuel 1041 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	21	20	19.9	19.6	19.5	19.7	19.5	19.5
Cetane Index	45.5	45.1	45.4	44.9	45	44.9	44	43.6
Density (g/mL)	0.8044	0.8018	0.8032	0.803	0.8024	0.8036	0.8031	0.8056
Distil. 10% (°C)	175.3	172.6	174.9	175.5	174.1	178.7	176.9	178.9
Distil. 20% (°C)	183.7	180	182.9	183.2	182	186.3	183.7	186.5
Distil. 50% (°C)	206.2	202.5	204.7	204.5	203.3	206.6	204.3	206.5
Distil. 90% (°C)	247.7	245	244.4	242.7	242.4	241.9	241.2	241.2
Flash Point (°C)	47.7	46.8	47.5	48	47.3	50.4	49.3	51
Freeze Point (°C)	-50.1	-52.1	-51.6	-51.6	-52.2	-51.2	-51.6	-49
H-Content (%)	13.7	13.7	13.7	13.7	13.7	13.7	13.7	13.7
Viscosity -20°C (cSt)	4.4	4.3	4.2	4.1	4.1	4.1	4	4.2

Table A8. Chemometic model data output for Jet fuel 890 across the test temperature range.

	-35°C	-18°C	0°C	21°C	27°C	39°C	49°C	58°C
Aromatics (%)	16.3	17.9	15.7	17.1	17.2	17.0	17.8	18.3
Cetane Index	47	47	46	46	46	46	47	47
Density (g/mL)	0.7980	0.7999	0.7967	0.8000	0.8014	0.8014	0.8029	0.8025
Distil. 10% (°C)	172.1	172.1	169.9	177.7	179.7	177.6	184.1	186.9
Distil. 20% (°C)	181.2	181.7	177.9	186.8	188.7	186.7	193.5	196.3
Distil. 50% (°C)	199.5	201.4	196.7	204.0	205.6	203.8	210.1	212.2
Distil. 90% (°C)	238.2	242.6	236.5	239.0	238.8	237.6	239.9	240.2
Flash Point (°C)	45.2	45.7	44.7	49.7	50.6	49.5	52.9	54.4
Freeze Point (°C)	-49.5	-47.6	-49.6	-48.2	-47.3	-48.0	-46.7	-46.0
H-Content (%)	13.9	13.9	13.9	13.9	13.9	13.9	13.9	13.9
Viscosity -20°C (cSt)	4.3	4.5	4.1	4.2	4.2	4.1	4.1	4.2

Table A9. Chemometic model data output for Jet fuel 890 across the test temperature range.

Appendix B

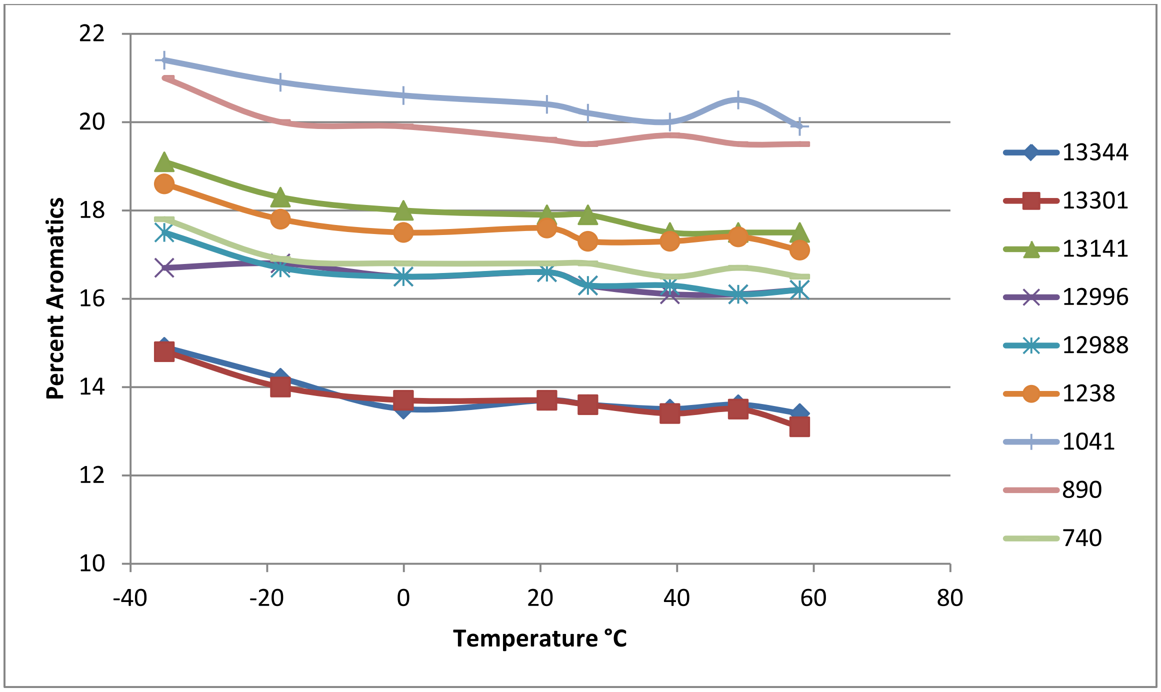

Figure B1. Percent aromatics predicted over -35ºC to 58ºC temperature range.

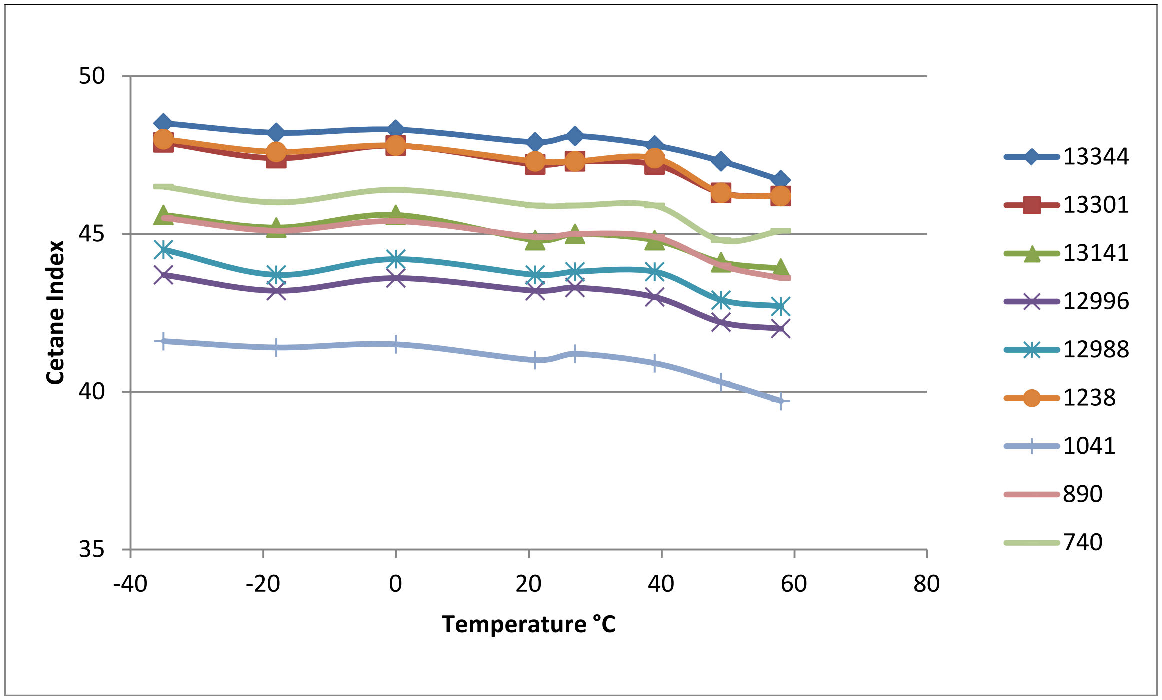

Figure B2. Calculated Cetane Index predicted over -35ºC to 58ºC temperature range.

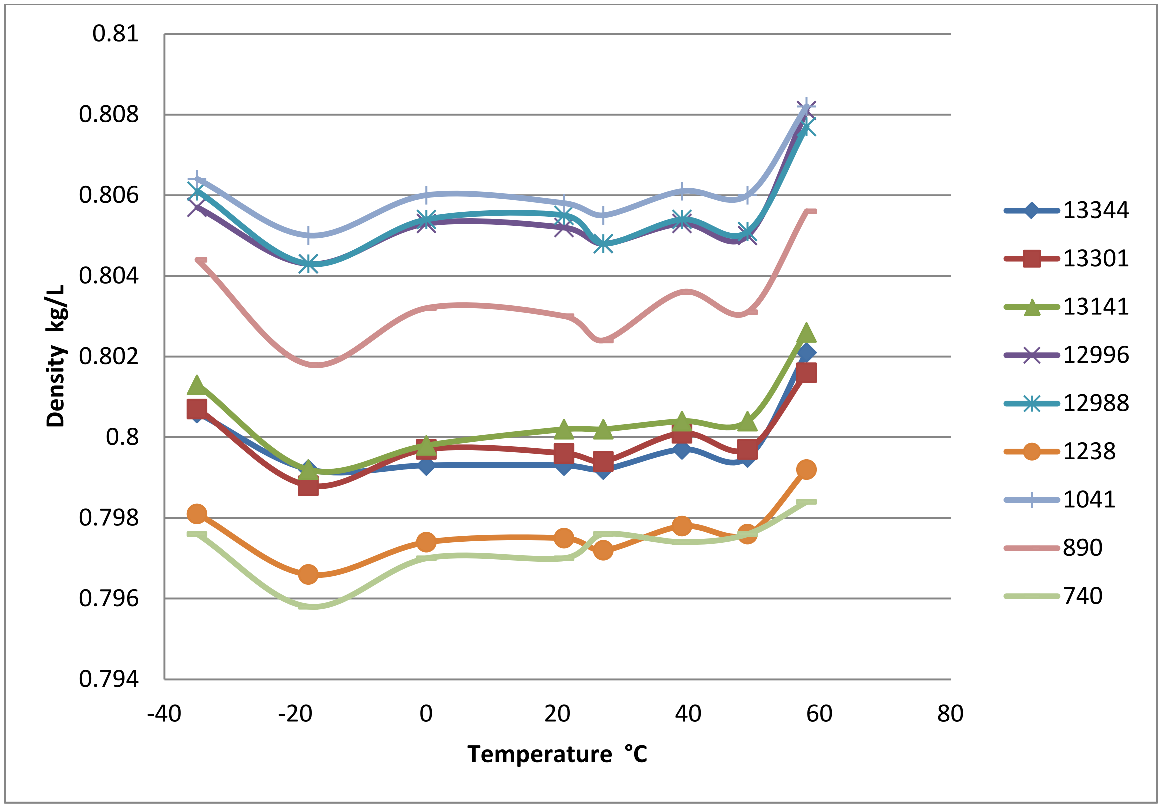

Figure B3. Fuel density in kg/L predicted over -35ºC to 58ºC temperature range.

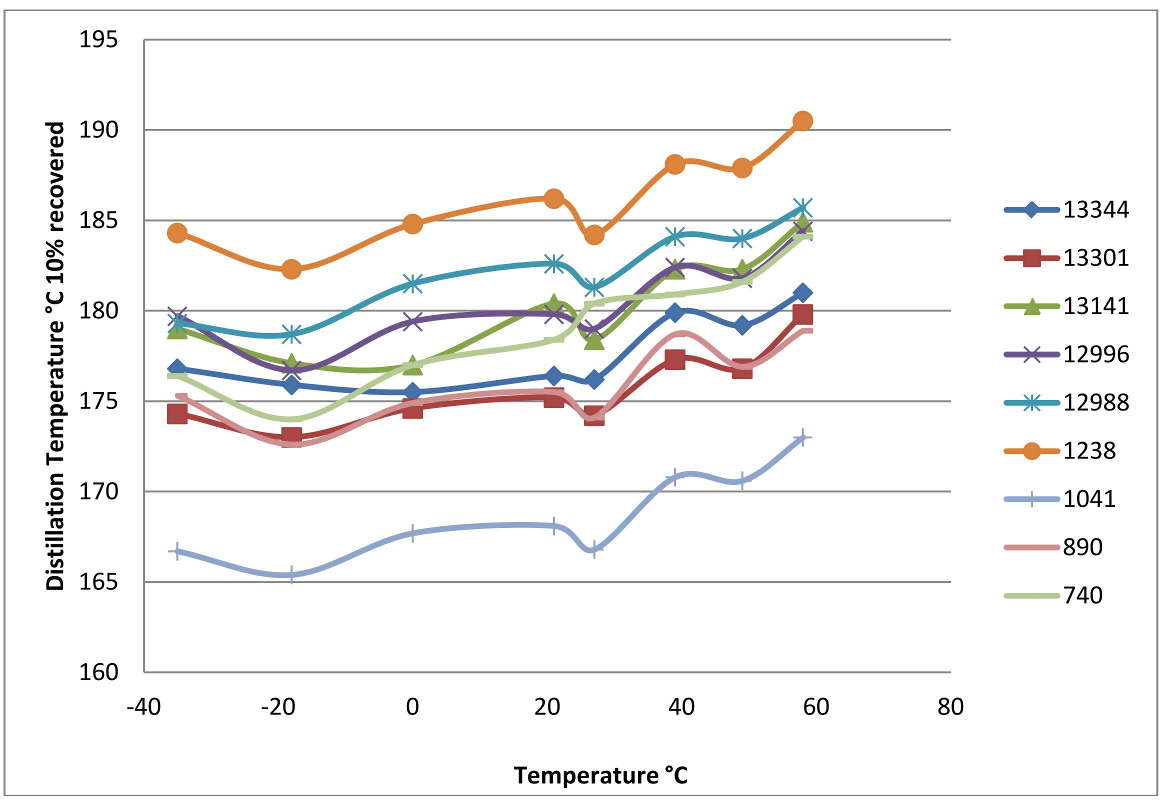

Figure B4. Distillation Temperature in ºC at 10% recovered predicted over -35ºC to 58ºC temperature range.

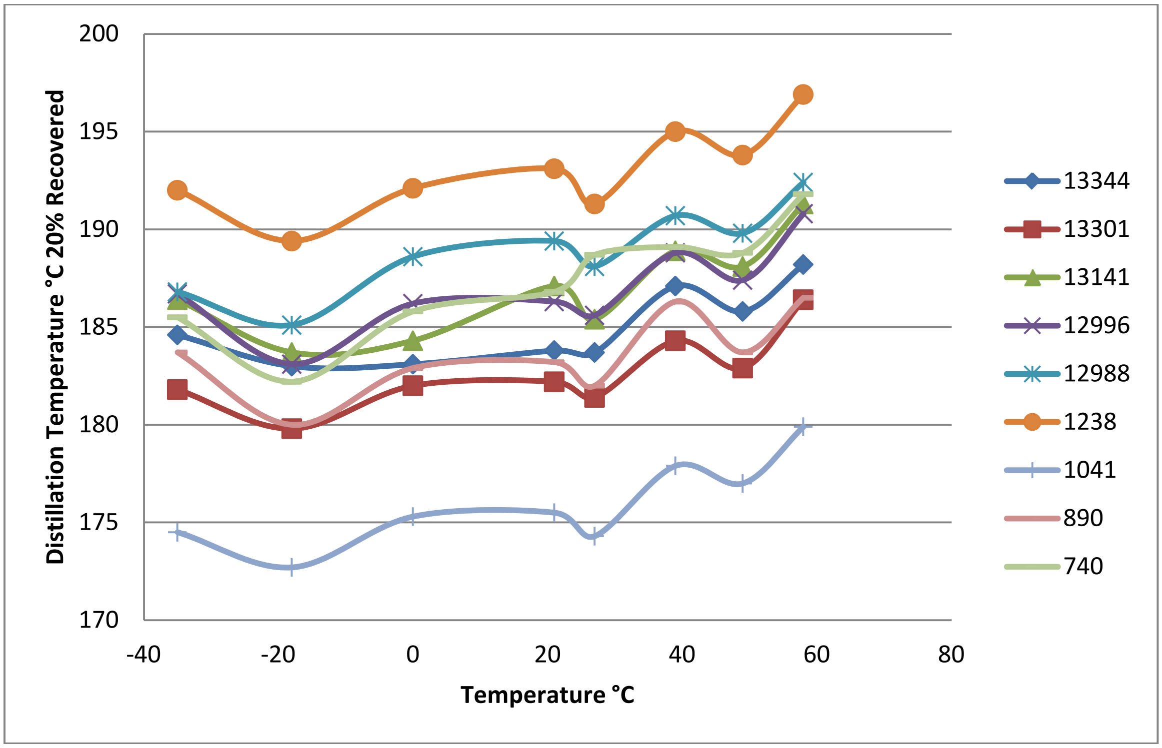

Figure B5. Distillation Temperature in ºC at 20% recovered predicted over -35ºC to 58ºC temperature range.

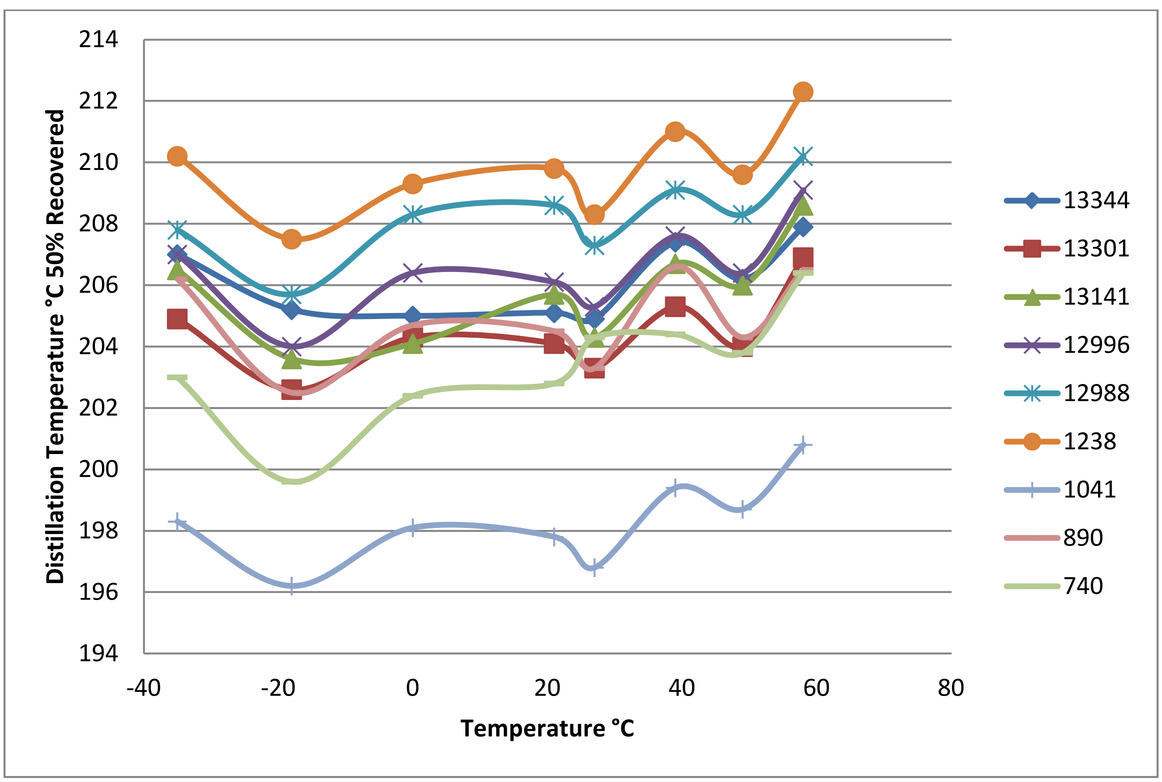

Figure B6. Distillation Temperature in ºC at 50% recovered predicted over -35ºC to 58ºC temperature range.

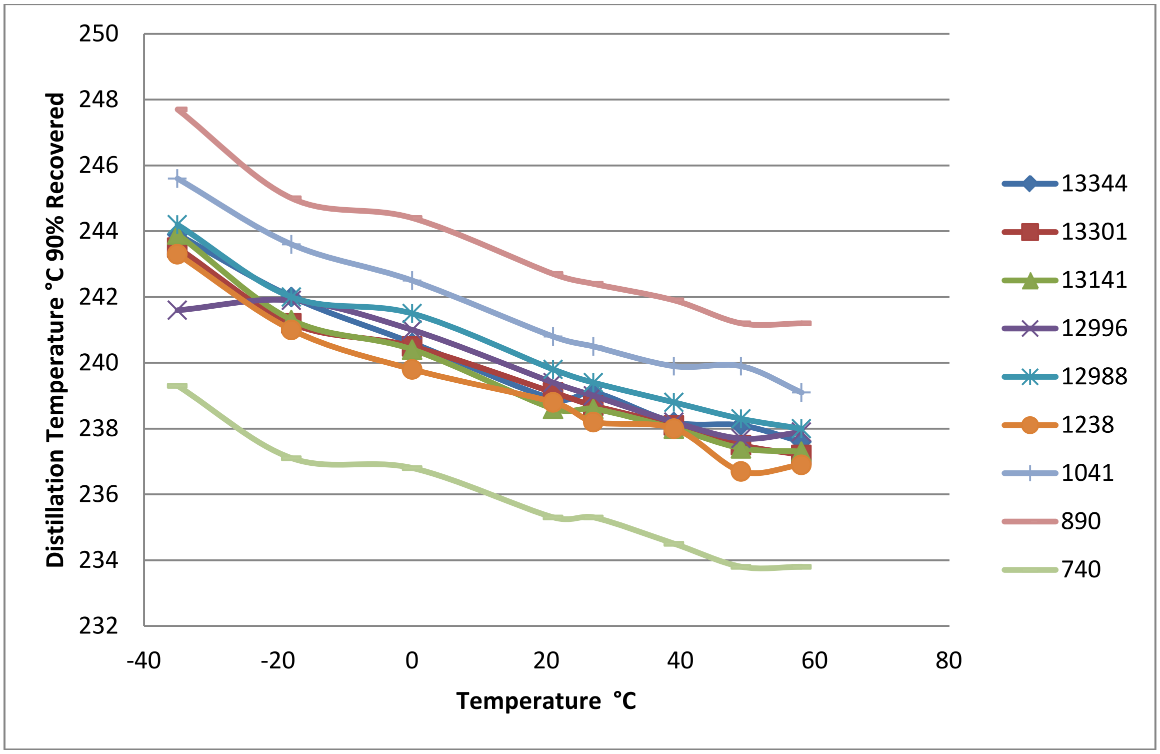

Figure B7. Distillation Temperature in ºC at 90% recovered predicted over -35ºC to 58ºC temperature range.

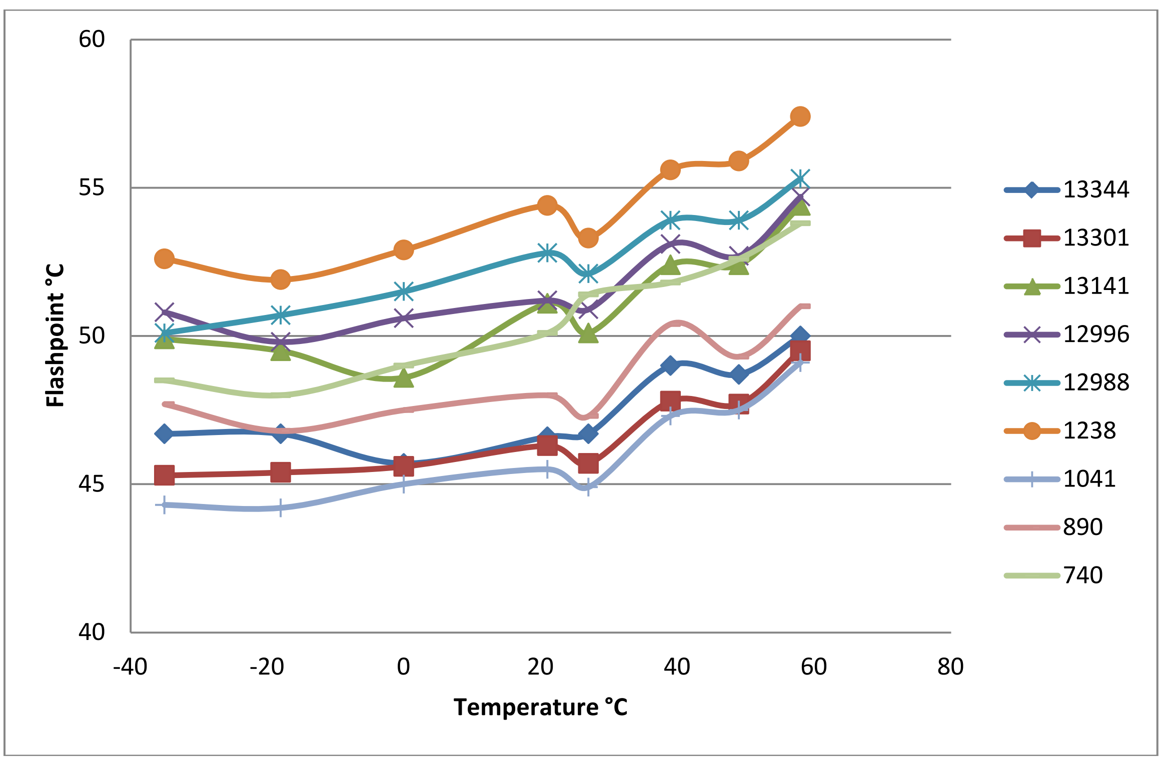

Figure B8. Flashpoint predicted over -35ºC to 58ºC temperature range.

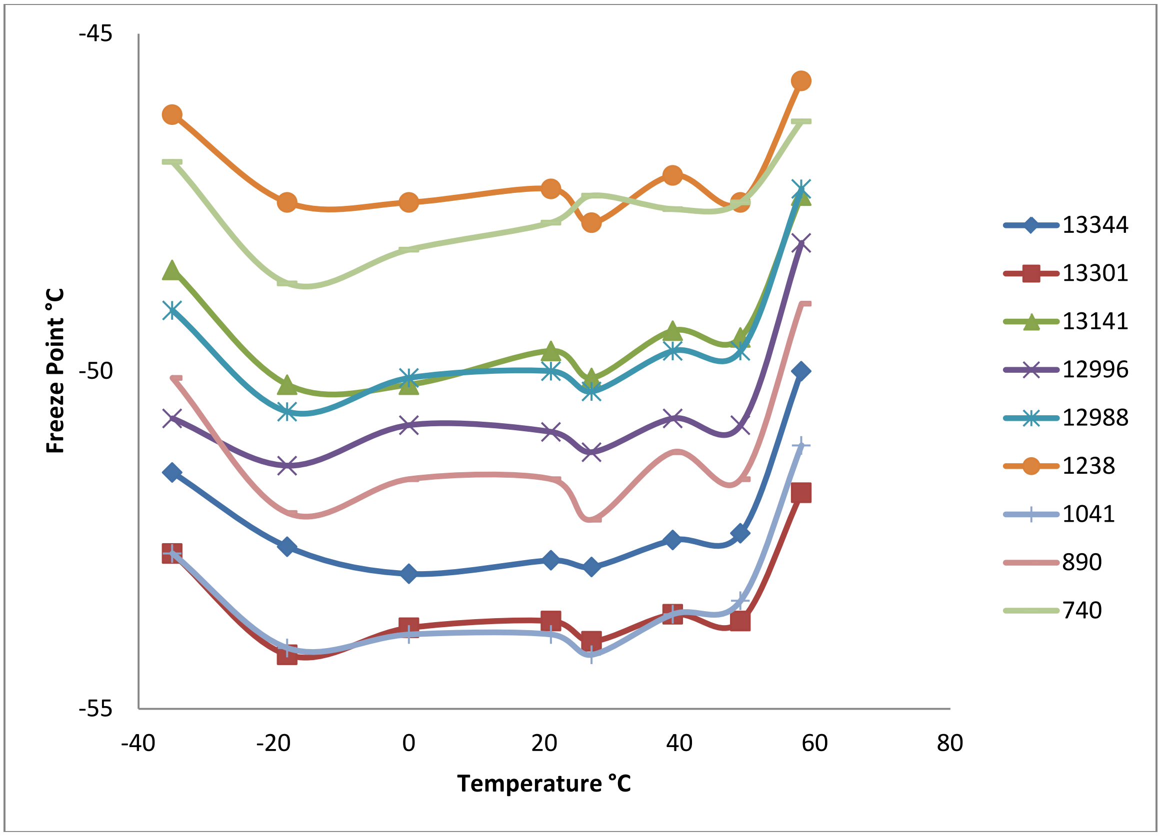

Figure B9. Freezing point predicted over -35ºC to 58ºC temperature range.

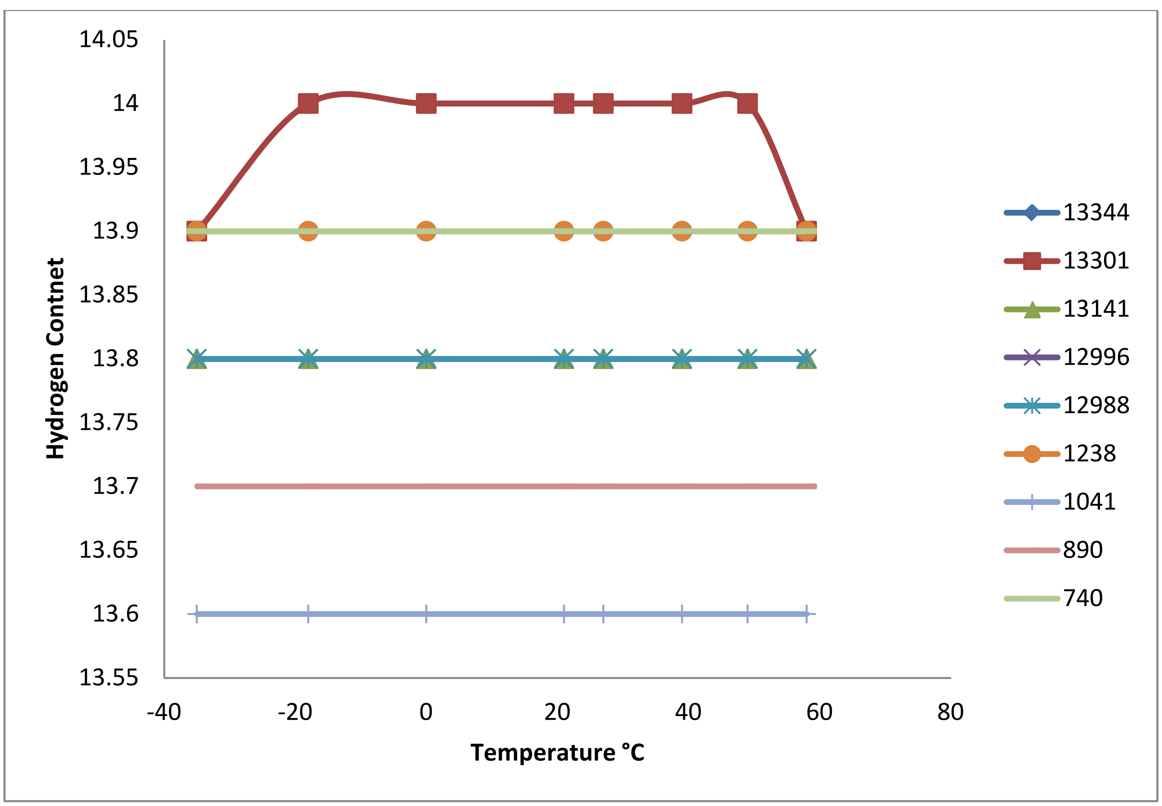

Figure B10. Hydrogen content predicted over -35ºC to 58ºC temperature range.

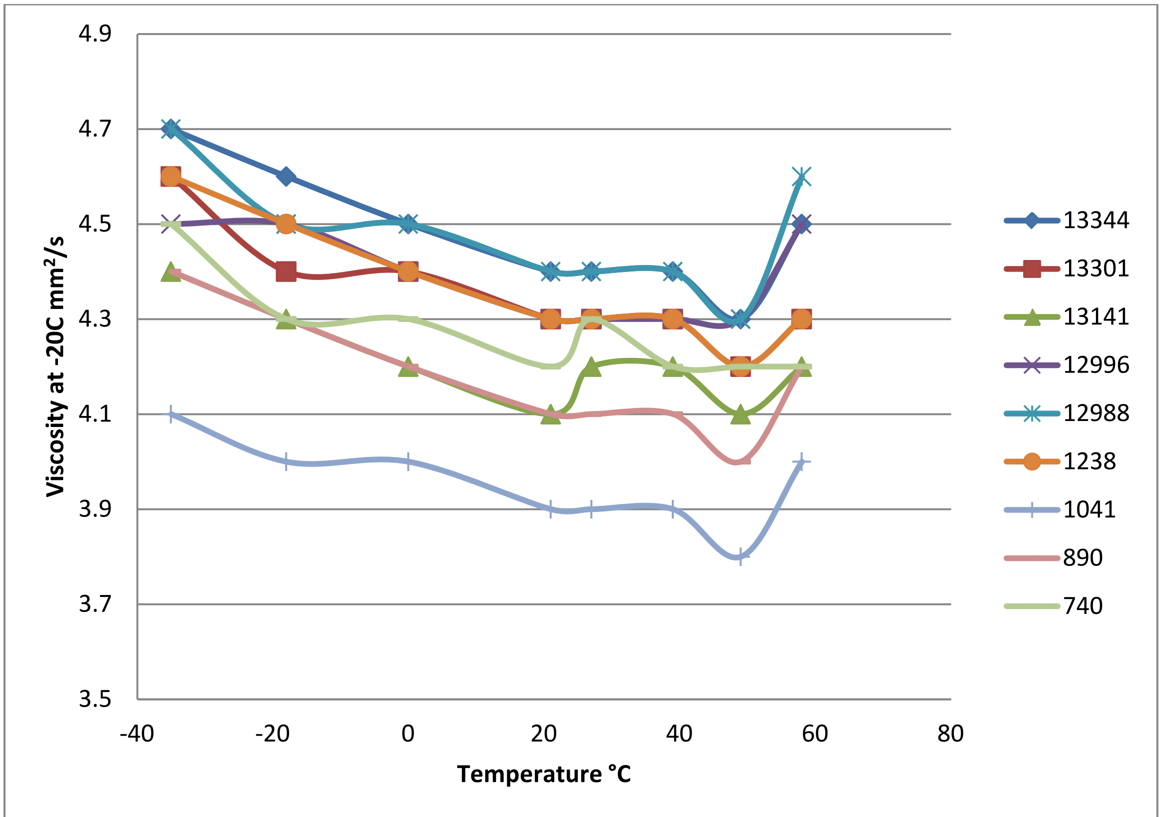

Figure B11. Viscosity in mm^2/s at -20ºC predicted over -35ºC to 58ºC temperature range.

List of Symbols, Abbreviations, and Acronyms

°C	degree(s) Celsius
CPD	Capabilities Production Document
cSt	centistokes
Distil.	temperature at distillation boiling point
g	grams
JP-5	Jet Propellant 5
JP-8	Jet Propellant 8
kg	kilogram
L	Liter
mL	milliliter
mm	millimeter
NIR	Near Infrared
nm	nanometer
ORD	Operational Requirements Document
PLS	Partial Least Squares
PTK	Petroleum Test Kit
TARDEC	Tank Automotive Research Development and Engineering Center
s	second
SNV	Standard Normal Variate